Diethyl ether

	outy, outor	
60-29-7	DTXSID30	21720

Model Performance

Model	Data

Weighted KNN model

5-fold CV (7	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.72	51.8	0.74	50.3	0.73	52.7	

Model Results

Predicted value: -114 °C

Global applicability domain: Inside

Local applicability domain index: 8.63e-01

Confidence level: 8.47e-01

Nearest Neighbors from the Training Set

Image not found

Diethyl ether Measured: -116 Predicted: -114

Image not found

Butane, 1-methoxy-Measured: -116 Predicted: -118

Image not found

Propane, 1-ethoxy-Measured: -128 Predicted: -118

Image not found

Methyl tert-butyl ether Measured: -109 Predicted: -102